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Vivek Shenoy

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The views, opinions and/or findings contained in this report are those of the author(s) and should not contrued as an official Department of the Army position, policy or decision, unless so designated by other documentation.

14. ABSTRACT

This reports describes the progress made in the second phase of the project after the PI moved from Brown to the University of Pennsylvania. The breakthrough results obtained are 1) prediction and subsequent experimental observation of strain induced changes in electronic structure of TMD materials 2) Prediction and experimental observation of using defects in 2D materials to enhance charge storage capacity and 3) Tuning the thermal conductivity of 2D materials through defect and strain engineering and 4) Develeopment of multiscale methods to simulate the growth of 2D materials. The work at Penn lead to 12 publications, inclduing papers in Nature

15. SUBJECT TERMS

2D Materials, Strain Engineering, MultiScale Modeling

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Report Title

Final Report: 9.4: Multi-scale modeling, design strategies and physical properties of 2D composite sheets

ABSTRACT

This reports describes the progress made in the second phase of the project after the PI moved from Brown to the University of Pennsylvania. The breakthrough results obtained are 1) prediction and subsequent experimental observation of strain induced changes in electronic structure of TMD materials 2) Prediction and experimental observation of using defects in 2D materials to enhance charge storage capacity and 3) Tuning the thermal conductivity of 2D materials through defect and strain engineering and 4) Develeopment of multiscale methods to simulate the growth of 2D materials. The work at Penn lead to 12 publications, including papers in Nature Materials, Nature Communications and Nano Letters.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received		Paper
01/15/2015	6.00	Dibakar Datta, Junwen Li, Nikhil Koratkar, Vivek B. Shenoy. Enhanced lithiation in defective graphene, Carbon, (12 2014): 0. doi: 10.1016/j.carbon.2014.08.068
01/15/2015	12.00	Esteban Meca, John Lowengrub, Hokwon Kim, Cecilia Mattevi, Vivek B. Shenoy. Epitaxial Graphene Growth and Shape Dynamics on Copper: Phase-Field Modeling and Experiments, Nano Letters, (11 2013): 0. doi: 10.1021/nl4033928
01/15/2015	11.00	Damien Voiry, Maryam Salehi, Rafael Silva, Takeshi Fujita, Mingwei Chen, Tewodros Asefa, Vivek B. Shenoy, Goki Eda, Manish Chhowalla. Conducting MoS2 Nanosheets as Catalysts for Hydrogen Evolution Reaction, Nano Letters, (12 2013): 0. doi: 10.1021/nl403661s
01/15/2015	10.00	Dibakar Datta, Junwen Li, Vivek B. Shenoy. Defective Graphene as a High-Capacity Anode Material for Na- and Ca-Ion Batteries, ACS Applied Materials & Interfaces, (02 2014): 0. doi: 10.1021/am404788e
01/15/2015	9.00	Sina Najmaei, Xiaolong Zou, Dequan Er, Junwen Li, Zehua Jin, Weilu Gao, Qi Zhang, Sooyoun Park, Liehui Ge, Sidong Lei, Junichiro Kono, Vivek B. Shenoy, Boris I. Yakobson, Antony George, Pulickel M. Ajayan, Jun Lou. Tailoring the Physical Properties of Molybdenum Disulfide Monolayers by Control of Interfacial Chemistry, Nano Letters, (03 2014): 0. doi: 10.1021/nl404396p
01/15/2015	8.00	Rahul Mukherjee, Abhay V. Thomas, Dibakar Datta, Eklavya Singh, Junwen Li, Osman Eksik, Vivek B. Shenoy, Nikhil Koratkar. Defect-induced plating of lithium metal within porous graphene networks, Nature Communications, (4 2014): 0. doi: 10.1038/ncomms4710
01/15/2015	7.00	Dequan Er, Junwen Li, Michael Naguib, Yury Gogotsi, Vivek B. Shenoy. Ti3C2 MXene as a High Capacity Electrode Material for Metal (Li, Na, K, Ca) Ion Batteries, ACS Applied Materials & Interfaces, (07 2014): 0. doi: 10.1021/am501144q
10/15/2013	1.00	Nikhil V. Medhekar, Vivek B. Shenoy, Junwen Li. Bonding Charge Density and Ultimate Strength of Monolayer Transition Metal Dichalcogenides, The Journal of Physical Chemistry C, (08 2013): 0. doi: 10.1021/jp403986v
10/15/2013	2.00	Manish Chhowalla, Hisato Yamaguchi, Junwen Li, Damien Voiry, Rafael Silva, Diego C. B. Alves, Takeshi Fujita, Mingwei Chen, Tewodros Asefa, Vivek B. Shenoy, Goki Eda. Enhanced catalytic activity in strained chemically exfoliated WS2 nanosheets for hydrogen evolution, Nature Materials, (07 2013): 0. doi: 10.1038/nmat3700
10/15/2013	3.00	Qing-Xiang Pei, Yong-Wei Zhang, Zhen-Dong Sha, Vivek B. Shenoy. Tuning the thermal conductivity of silicene with tensile strain and isotopic doping: A molecular dynamics study, Journal of Applied Physics, (07 2013): 1. doi: 10.1063/1.4815960
10/15/2013	4.00	J. Aarts, Inrok Hwang, Sungtaek Oh, Jin Sik Choi, Dmitri Strukov, Taekjib Choi, Bae Ho Park, Vivek B. Shenoy, Peter Maksymovych, Sergei V. Kalinin, Nicole Benedek, Yunseok Kim, Simon J. Kelly, Anna Morozovska, Ehsan Kabiri Rahani, Evgheni Strelcov, Eugene Eliseev, Stephen Jesse, Michael D. Biegalski, Nina Balke. Mechanical Control of Electroresistive Switching, Nano Letters, (08 2013): 4068. doi: 10.1021/nl401411r

10/15/2013	5.00	Vivek B. Shenoy, David H. Gracias. Self-folding thin-film materials: From nanopolyhedra to graphene origami, MRS Bulletin, (09 2012): 0. doi: 10.1557/mrs.2012.184

TOTAL: **12**

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received Paper

TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Number of Presentations: 0.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received Paper

TOTAL:

Number of Manuscripts:

Books

Received Book

TOTAL:

Received Book Chapter

TOTAL:

Patents Submitted

Patents Awarded

Awards

Graduate Students

NAME	PERCENT_SUPPORTED	Discipline
Dibakar Datta	1.00	
Dequan Er	1.00	
FTE Equivalent:	**2.00**	
Total Number:	**2**	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
Vivek Shenoy	0.50	
FTE Equivalent:	**0.50**	
Total Number:	**1**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED	Discipline
Kevin Zhai	1.00	Materials Science
Joshua Douglas	1.00	Materials Science
FTE Equivalent:	**2.00**	
Total Number:	**2**	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 2.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:..... 2.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:..... 2.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):..... 2.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:..... 0.00

Names of Personnel receiving masters degrees

NAME
Xuan Cao
Total Number: **1**

Names of personnel receiving PHDs

NAME
Dibakar Datta
Total Number: 1

Names of other research staff

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

The breakthrough results obtained are 1) prediction and subsequent experimental observation of strain induced changes in electronic structure of TMD materials 2) Prediction and experimental observation of using defects in 2D materials to enhance charge storage capacity and 3) Tuning the thermal conductivity of 2D materials through defect and strain engineering and 4) Develeopment of multiscale methods to simulate the growth of 2D materials and 5) Prediction and validation of methods to engineer interfaces in 2D materials. The abstracts of all the papers have been uploaded along with this report. The work at Penn lead to 12 publications, including papers in Nature Materials, Nature Communications and Nano Letters. We collaborated with ARO PI, Dr. Ajayan and published a paper on 2D materials with his group. We have also been regularly interacting with Madan Dubey's group at ARO. In the last year of the projected we presented two talks at ARO and one at APG.

Technology Transfer